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Theoretical analysis on the band structure variance of the electron doped 1111 iron-based superconductors

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Abstract

We perform first principles band calculation of electron doped iron-based superconductors adopting the virtual crystal approximation. We find that when electrons are doped by element substitution in the blocking layer, the band structure near the Fermi level is affected due to the increase of the positive charge in the layer. On the other hand, when Fe in the conducting layer is substituted by Co, the band structure is barely affected. This difference should be a key factor in understanding the phase diagram of the heavily doped electron doped systems $LnFeAsO_{1-x}H_x$.

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Keywords: iron-based superconductors, virtual crystal approximation, doping effect, theoretical analysis

1. Introduction

Recently, interesting phase diagrams have been obtained for the 1111 iron-based superconductors $LnFeAsO_{1-x}H_x$ (*Ln*=La, Sm, etc.), where electrons are doped into the conducting FeAs layer by partially substituting oxygen in the blocking *Ln*O layer by hydrogen[2]. In these materials, spin fluctuation and superconductivity are observed even in the heavily electron doped regime x~0.4[2,3], where the characteristic hole Fermi surfaces are expected to be wiped

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out within a rigid band picture. Recent theoretical studies have revealed that the electronic structure actually varies with doping [4,5], which can be the origin of the lasting spin fluctuation and superconductivity. On the other hand, in materials in which electrons are doped by partially substituting Fe in the conducting layer by Co, such as $La(Fe_{1-x}Co_x)AsO$[6], $Ba(Fe_{1-x}Co_x)_2As_2$[7], etc., spin fluctuation and superconductivity is lost around x=0.2[8]. This seems to suggest that a rigid band picture holds in these materials[9]. The understanding of the difference between blocking and conducting layer element substitutions should lead to further understanding of the occurrence of high T_c superconductivity in $LnFeAsO_{1-x}H_x$.

In the present paper, we study the origin of this difference theoretically. We perform first principles band calculation of $LaFe_{1-x}Co_xAsO$ and $LaFeAsO_{1-x}F_x$ using the virtual crystal approximation, and discuss the doping dependence of the band structure for the two systems. As for the former material, a more sophisticated supercell analysis has been done in a previous study[10], with which the present result is consistent. The aim of the present study is to compare the two ways of electron doping within the same (more simple) method, i.e., the virtual crystal approximation. We also study the band structure of $Ba(Fe_{1-x}Co_x)_2As_2$ for comparison.

2. Doping dependence of band structure

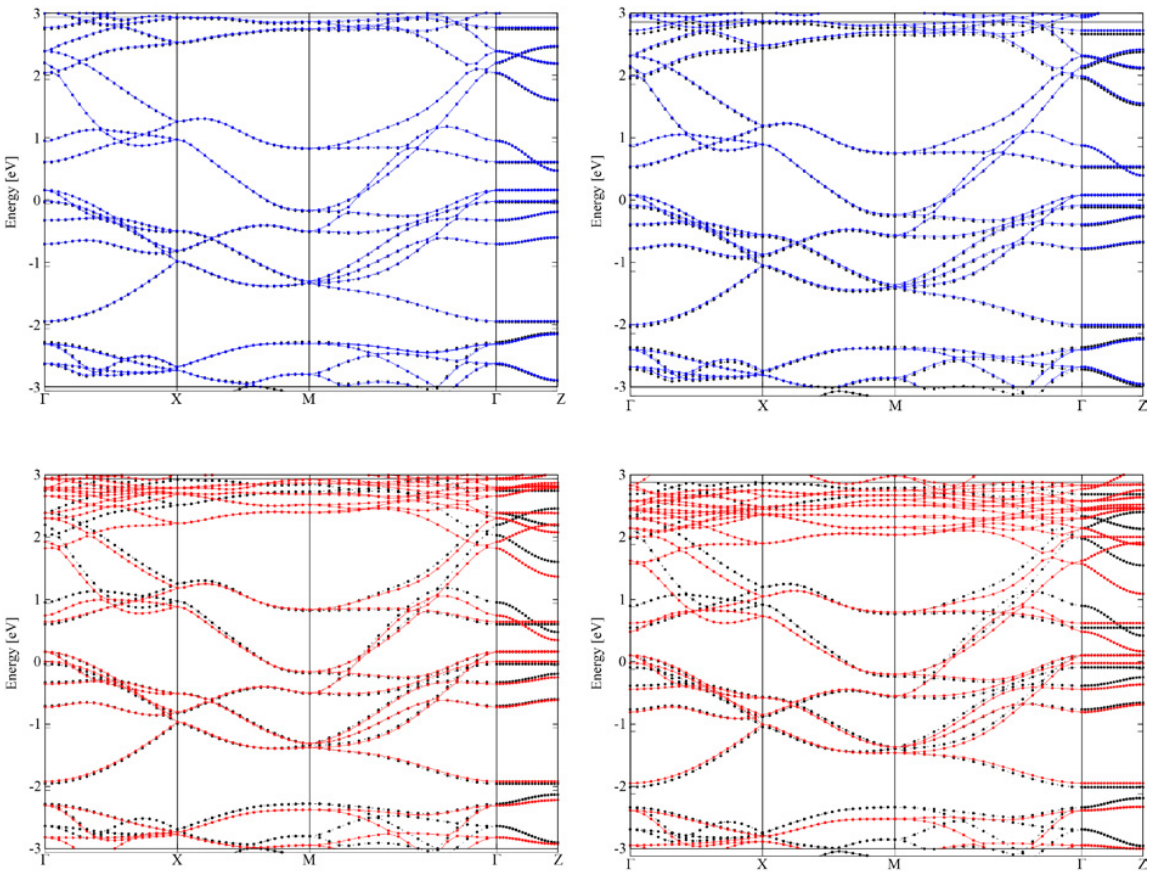

Fig. 1. The band structure of $LaFe_{1-x}Co_xAsO$ (blue) and $LaFeAsO_{1-x}F_x$ (red) for x=0.1(left) and x=0.2(right). The band structure of the undoped mother compound is also shown for comparison (dashed lines). The Fermi energy is shifted by doping, but in order to focus on the band structure variance with doping, we align, for doped and undoped cases, the energies of the two degenerate bands at the Γ point near E=0. Note that the doped and the undoped band structure is barely resolved for the case of Co doping.

First, we perform first principle band calculation using VASP package[11,12] for cobalt doped $LaFe_{1-x}Co_xO$ and fluorine doped $LaFeAsO_{1-x}F_x$ for the doping rate of x=0.1 and 0.2. We fix the lattice parameters to those determined experimentally for the mother compound LaFeAsO[1]. We adopt the virtual crystal approximation, in which the iron (oxygen) and cobalt (fluorine) pseudopotentials are mixed, thereby taking into account the effect of the increasing average valence on the substituted site by $+x$. Here we take the cutoff energy E_{cut}=550eV, 1000 k-points, and adopt GGA-PBE exchange correlation functional[13]. The comparison is given in Fig. 1, which shows that the blocking layer substitution ($LaFeAsO_{1-x}F_x$) affects the band structure around the Fermi energy, while the conducting layer substitution ($LaFe_{1-x}Co_xAsO$) has nearly no effect. This difference can be understood as follows. Substituting oxygen by fluorine increases positive charge in the blocking layer. It lowers the As 4p energy level and reduces the hybridization between As 4p and Fe 3d, so that the 3d-originated band structure near the Fermi level is affected. On the other hand, the conducting layer substitution does not introduce such a change in the charge distribution between conducting and blocking layers, so that the band structure is barely affected. In this case, the doping induces only the Fermi energy shift, so that a rigid band picture holds. The result for $LaFe_{1-x}Co_xAsO$ is consistent with a previous supercell study[10].

3. $Ba(Fe_{1-x}Co_x)_2As_2$

To confirm the generality of the present result, we study another material where electrons are doped by conducting layer substitution, a 122 system $Ba(Fe_{1-x}Co_x)_2As_2$. Fig. 2 shows the band structure of $Ba(Fe_{1-x}Co_x)_2As_2$ for x=0, x=0.1 and 0.2 obtained by adopting the lattice structure of $BaFe_2As_2$[14] and adopting the virtual crystal approximation. It shows that the Co doping does not change the band structure as in $LaFe_{1-x}Co_xAsO$. This further confirms our conclusion that the conducting layer substitution barely affects the band structure near the Fermi energy.

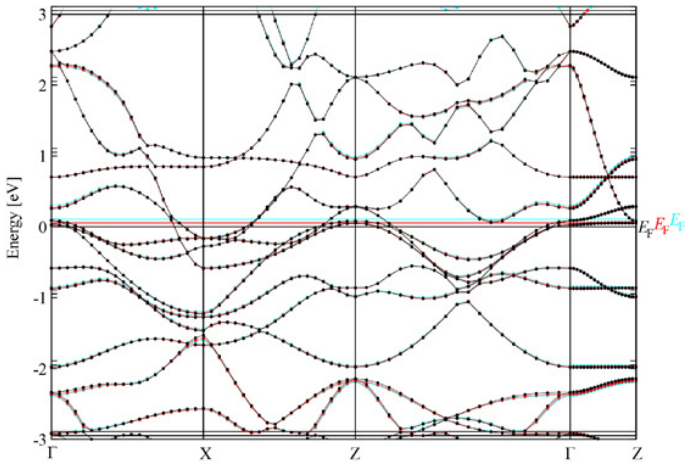

Fig. 2. Band structure of $Ba(Fe_{1-x}Co_x)_2As_2$. for x = 0.1 (red) and x=0.2 (cyan). The band structure of the undoped material is also shown for comparison (black). For all three doping rates, we align the energies of the two degenerate bands at the Γ point. The three sets of band structure are barely resolved.

4. Conclusion

In conclusion, we performed first principle band calculation of three electron doped materials, $LaFe_{1-x}Co_xAsO$, $LaFeAsO_{1-x}F_x$ and $Ba(Fe_{1-x}Co_x)_2As_2$ adopting the virtual crystal approximation. We find significant difference between blocking layer and conducting layer element substitutions. While the conducting layer substitution has small effect on the band structure, the blocking layer substitution affects the bands around the Fermi energy. This difference should be a key factor in understanding the phase diagram of the heavily electron doped $LnFeAsO_{1-x}H_x$

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